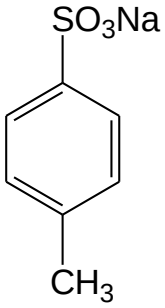
SIDS INITIAL ASSESSMENT PROFILE

CAS No.	657-84-1
Chemical Name	Sodium *p*-toluenesulfonate
Structural Formula	

SUMMARY CONCLUSIONS OF THE SIAR

Analogue rationale

At SIAM 21 in 2005, the Hydrotropes category was discussed and approved. The Hydrotropes category covers "toluene sulfonic acid, sodium salt", "xylene sulfonic acid, sodium salt" and "cumene sulfonic acid, sodium salt". This category also includes isomeric forms (ortho, meta, and/or para) of the respective sulfonic acid salts (sodium, ammonium, calcium and potassium). Although "sodium *p*-toluenesulfonate" is one of the category member, the SIDS documents of sodium *p*-tolunesulfonate are prepared separately as the sponsor country has obtained some new test (or experimental) data on this chemical. New SIDS information on sodium *p*-toluenesulfonate is introduced in this document, however, the evaluation of the endpoints of skin/eye irritation and sensitization were read across from the Hydrotopes category document.

Physical-chemical properties

Sodium *p*-toluenesulfonate is white crystal solid with a melting point of > 300 °C at 1013 hPa. Although an estimated boiling point is 533 °C, sodium *p*-toluenesulfonate may decompose before reaching this temperature. Vapour pressure and partition coefficient (Log K_{ow}) are estimated to be of 3.51×10^{-9} Pa at 25 °C and -2.40 respectively. Measured and estimated values for water solubility are > 250 g/L at 20 °C and 1000 g/L at 25 °C respectively.

Human Health

Sodium *p*-toluenesulfonate-^{35}S was rapidly absorbed and excreted by rats and dogs given an oral or intraperitoneal administration. Both species excreted the radioactivity primarily in the urine (82–85 % of the dose) and, to a lesser extent, in the feces (13–18 % of the dose). In dogs, sodium *p*-toluenesulfonate-^{35}S had a biological half-life in the plasma of 75 min. Only the unaltered *p*-toluenesulfonate-^{35}S moiety was detected chromatographically in the excreta of both species.

The oral LD_{50} values in rats for sodium *p*-toluenesulfonate were greater than 2000 mg/kg bw in both sexes [OECD TG 401]. Sodium *p*-toluenesulfonate administered orally caused diarrhea at a dose of 2000 mg/kg bw. No valid studies were available for sodium *p*-toluenesulfone for acute dermal and acute inhalation studies.

In the Hydrotropes Category, calcium xylene sulfonate and sodium cumene sulfonate are concluded to be non skin irritants. However,sodium *p*-toluenesulfonate may have a potential to cause skin and eye irritation in animals due to high pH(9.6) in aqueous solution, although no direct experimental data are available.

No studies of respiratory tract sensitisation on sodium *p*-toluenesulfonate are available. There is no indication of skin sensitization for toluenesulfonic acid, sodium salt (ortho, meta and/or para) in

guinea pigs according to the SIDS document of Hydrotopes category. It is therefore considered that sodium *p*-toluenesulfonate is not a skin sensitizer.

In a repeated-dose oral toxicity study in rats [OECD TG 407], sodium *p*-toluenesulfonate was administered orally by gavage to male and female rats (5 or 10 animals/sex/group) for 28 days at doses of 0, 100, 300 and 1000 mg/kg bw/day. As recovery groups, 5 animals/sex from the control and high-dose groups were sacrificed at the end of the recovery period (day 43). No deaths were observed in any group. There were no treatment-related changes in clinical signs, body weight, food intake and hematological or biochemical examination in either sex. An increase in urine specific gravity observed in male groups at 1000 mg/kg bw/day was considered to have no toxicological significance because no other relevant changes were found. Based on these results, the NOAEL for this repeated-dose oral toxicity study was found to be 1000 mg/kg bw/day in both male and female rats.

In an oral reproductive and developmental toxicity screening test (OECD TG 421: doses of 0, 100, 300 and 1000 mg/kg bw/day), diarrhea and soft feces were observed as systemic general toxicity at the dose of 1000 mg/kg in parental male and female animals. And inflammatory cellular infiltration of lamina propria and squamous cell hyperplasia in the stomach limiting ridge were observed in the male group at 1000 mg/kg bw/day. The NOAEL of systemic toxicity for this reproductive and developmental toxicity screening test was found to be 300 mg/kg bw/day.

The overall NOAEL of sodium p-toluenesulfonate for repeated dose oral toxicity was found to be 300 mg/kg bw/day in both male and female rats.

No data are available for the repeated-dose inhalation and dermal toxicity of sodium *p*-toluenesulfonate.

A bacterial reverse mutation assay using four strains of *Salmonella typhimurium* and an *Escherichia coli* strain, WP2 *uvrA* [OECD TG 471] on sodium *p*-toluenesulfonate was negative both with and without metabolic activation. An *in vitro* chromosome aberration test using CHL/IU cells [OECD TG 473] was also negative with or without metabolic activation. Although there are no data available for *in vivo* mutagenicity on sodium *p*-toluenesulfonate, the chemical is not considered to be genotoxic *in vitro* based on negative outcomes in *in vitro* assays.

No data are available for the carcinogenicity of sodium *p*-toluenesulfonate.

In a reproductive and developmental toxicity screening test in rats [OECD TG 421], sodium *p*-toluenesulfonate was administered orally by gavage at doses of 0, 100, 300 and 1000 mg/kg bw/day. Then both the reproductive performance of parental animals and the development and growth of F1 offspring were examined. There was no significant effect of sodium p-toluenesulfonate on the numbers of total offspring and live offspring, sex ratio, live birth index, viability index or body weight, and no compound-related abnormality was found in external features, clinical signs or autopsy findings of offspring up to 1000 mg/kg bw/day, the highest dose tested, while some toxic effects on parental animals (diarrhea, soft feces, etc.) were observed at 1000 mg/kg bw/day. Thus the NOAEL for reproductive and developmental toxicity was considered to be 1000 mg/kg bw/day in rats.

Environment

Sodium *p*-toluenesulfonate is dissociated into sodium ion and *p*-toluenesulfonate ion in water. Hydrolysis test of *p*-toluenesulfonate according to OECD Test-guideline 111 shows no hydrolysis at pH4, pH7 and pH9 at 50 °C for 5 days. *p*-Toluenesulfonate is readily biodegradable under aerobic conditions with BOD biodegradability of 93 % in 3 weeks (equivalent to OECD TG301C). Bioaccumulation potential of sodium *p*-toluenesulfonate seems to be low based on an estimated Log K_{ow} of -2.40, which is supported by a calculated BCF value of 3.16with BCFWIN.

In the atmosphere, indirect photo-oxidation of sodium *p*-toluenesulfonate by reaction with hydroxyl radicals is estimated to result in a half-life of 8.8 days. However, photo-degradation as an environmental fate mechanism may not be important as sodium *p*-toluenesulfonate is not volatile.

Sodium *p*-toluenesulfonate has an estimated Henry's law constant of 2.83×10^{-4} $Pa.m^3$/mole at 25 °C, which suggests that volatilization of sodium *p*-toluenesulfonate from the water phase is expected to be negligible. Level III fugacity model shows that sodium *p*-toluenesulfonate will distribute mainly to the water compartment (99.8 %) with minor distribution to the sediment compartment (0.18 %) and negligible amounts in the air and soil compartments if released only to the water compartment.

The following acute toxicity test results have been determined for aquatic species:

Oryzias latipes:	96 h LC_{50} >100 mg/L (nominal)
Daphnia magna:	48 h LC_{50} >1,000 mg/L (nominal)
Pseudokirchneriella subcapitata:	72 h ErC_{50} > 1,000 mg/L (growth rate method, nominal)
Pseudokirchneriella subcapitata:	72 h EbC_{50} > 1,000 mg/L (AUG method, nominal)

The following chronic toxicity test results have been determined:

Daphnia magna:	21 d NOEC = 100 mg/L (nominal)
Pseudokirchneriella subcapitata:	72 h NOErC = 10 mg/L (growth rate method, nominal)
Pseudokirchneriella subcapitata:	72 h NOEbC = 10 mg/L (AUG method, nominal)

Exposure

In Japan, sodium *p*-toluenesulfonate was commercially produced and/or imported with an annual production volume of 100 tonnes – 1,000 tonnes in the fiscal year 2004. According to the SPIN database, the total use of sodium *p*-toluensulfonate was less than 10 tonnes in the Nordic countries in 2006. The worldwide production volume outside Japan is not available. Sodium *p*-toluenesulfonate is manufactured by neutralization of *p*-toluene sulfonate with sodium hydrate, here *p*-toluenesulfonate is made by sulfonation of *p*-toluene with sulphuric acid. Sodium *p*-toluenesulfonate is used as an anti-blocking agent in powder products, a solubilizer in detergents, and a dilution agent in dyes. No other information for the use pattern is obtained in the sponsor country.

In the sponsor country, manufacturing and formulation of sodium *p*-toluenesulfonate are conducted in a closed system. Even if a limited amount of sodium *p*-toluenesulfonate is released into the waste-water stream at production and processing sites, waste water stream is treated in the waste-water treatment plant. Furthermore, as sodium *p*-toluenesulfonate is readily biodegradable, emission of sodium *p*-toluenesulfonate from the production and processing sites into the environment is anticipated to be low. No monitoring data from production and processing sites are available in the sponsor country.

Sodium *p*-toluenesulfonate is used in consumer products, like detergents. Therefore, release from down-the-drain discharges following product use could lead to the environmental exposure into the surface water. However, as sodium *p*-toluenesulfonate is biodegradable and has limited potential for bio-accumulation, long-term environmental exposure is not foreseen.

Occupational exposure through an inhalation of aerosol may be a concern, and inhalation of vapor is negligible due to very low vapor pressure. Dermal intake may also be negligible due to low $\log K_{ow}$.

As sodium *p*-toluenesulfonate is used in consumer products, consumer exposure through dermal contact could exist. There are some potential intakes for incidental ingestion, inhalation and eye contact with sodium *p*-toluenesulfonate. However, these potential intakes may be mitigated by the fact that sodium *p*-toluenesulfonate is easily washed off through careful handling by consumers. No other information on consumer exposure is available.

RECOMMENDATION AND RATIONALE FOR THE RECOMMENDATION AND NATURE OF FURTHER WORK RECOMMENDED

Human Health: This chemical is currently of low priority for further work because of its low hazard profile.

Environment: This chemical is currently of low priority for further work because of its low hazard profile.